Quantum Discord and the Geometry of Bell-Diagonal States

Matthias D. Lang* and Carlton M. Caves
Center for Quantum Information and Control, University of New Mexico, MSC07-4220, Albuquerque, New Mexico 87131-0001, USA
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The set of Bell-diagonal states for two qubits can be depicted as a tetrahedron in three dimensions. We consider the level surfaces of entanglement and quantum discord for Bell-diagonal states. This provides a complete picture of the structure of entanglement and discord for this simple case and, in particular, of their nonanalytic behavior under decoherence. The pictorial approach also indicates how to show that discord is neither convex nor concave.

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Maintenance of quantum coherence is clearly important for quantum-information-processing protocols. Noise and decoherence, by turning pure states into mixed states, generally destroy quantum coherence. Efficient representation of quantum information requires that a quantum-information-processing system be composed of parts [1]. For multipartite systems, quantum coherence is related to nonclassical correlations between the parts.

One kind of nonclassical correlation is entanglement [2]. A pure quantum state is unentangled if it is a product of pure states for each part. A mixed state is unentangled (separable) if it can be written as an ensemble of such product states. Entanglement is the crucial resource for such quantum-information-processing protocols as quantum key distribution, teleportation, and superdense coding [2].

Operational measures of entanglement are notoriously difficult to calculate for mixed states; even the boundary between separability and entanglement is difficult to characterize. One can say, however, that the set of separable states is a convex set, is invariant under local unitary operations, and has dimension as large as the space of mixed states [2].

Separable states have nonzero measure in the space of all states [3]. In a decoherence process that involves decay to a separable equilibrium state that does not lie on the boundary between separability and entanglement, the decohering state will cross that boundary before reaching the equilibrium state. This phenomenon, dubbed "sudden death of entanglement" [4,5], is the generic expectation in view of the geometry of separable states.

Separable states can have nonclassical correlations even though they are unentangled. A state with only classical correlations, often called a classical state, is one that is diagonal in a product basis, for then the correlations are described by a joint probability distribution for classical variables of the parts. These purely classical states are a set of measure zero, as is suggested by the fact that any classical state can be perturbed infinitesimally to become nonclassical by making two of the eigenvectors infinitesimally entangled and is proved rigorously in [6].

A variety of measures have been proposed to quantify nonclassical correlations for bipartite systems [7–9], in ways that can be nonzero for separable, but nonclassical states. Nonclassical, but perhaps separable correlations have been related to exponential speedups in the "power-of-one-qubit" model [10] of mixed-state quantum computation [11], but the relation remains tenuous [12].

One can use decoherence mechanisms to explore the nooks and crannies of nonclassical-correlation measures. There is no sudden death [6], as is suggested by the absence of open sets of classical states, but the nonanalyticity of nonclassical measures points to the possibility of sudden changes in derivatives. Investigation of the behavior of nonclassical measures under decoherence has begun [5,13–15], with a focus on the action of decoherence within the class of two-qubit states that are diagonal in the Bell basis. This focus is motivated by the fact that entanglement measures and nonclassical-correlation measures can be calculated explicitly for the Bell-diagonal states, thus allowing one to determine how these measures change under decoherence.

The Bell-diagonal states are a three-parameter set, whose geometry, including the subsets of separable and classical subsets, can be depicted in three dimensions [2,16]. Level surfaces of entanglement and nonclassical measures can be plotted directly on this three-dimensional geometry. The result is a complete picture, for this simple case, of the structure of entanglement and nonclassicality. We suggest that it is more illuminating to use this picture to explain how measures of entanglement and nonclassicality change along the one-dimensional trajectories traced out by decohering states, rather than the other way around. Hence we review and expand the pictorial approach here.

The Bell-diagonal states of two qubits, A and B, have density operators of the form

$$\rho_{AB} = \frac{1}{4}\left(I + \sum_{j=1}^{3} c_j \sigma_j^A \otimes \sigma_j^B\right) = \sum_{a,b} \lambda_{ab} |\beta_{ab}\rangle\langle\beta_{ab}|, \quad (1)$$

where the σ_j's are Pauli operators. The eigenstates are the four Bell states $|\beta_{ab}\rangle \equiv (|0, b\rangle + (-1)^a |1, 1 \oplus b\rangle)/\sqrt{2}$, with eigenvalues

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$$\lambda_{ab} = \tfrac{1}{4}[1 + (-1)^a c_1 - (-1)^{a+b} c_2 + (-1)^b c_3]. \quad (2)$$

Any two-qubit state satisfying $\langle \sigma_j^A \rangle = 0 = \langle \sigma_j^B \rangle$, i.e., having maximally mixed marginal density operators $\rho_A = I/2 = \rho_B$, can be brought to Bell-diagonal form by using local unitary operations on the two qubits to diagonalize the correlation matrix $\langle \sigma_j^A \otimes \sigma_k^B \rangle$.

A Bell-diagonal state is specified by a 3-tuple (c_1, c_2, c_3). The density operator ρ_{AB} must be a positive operator, i.e., $\lambda_{ab} \geq 0$; the resulting region of Bell-diagonal states is the state tetrahedron $\mathcal{T}$ in Fig. 1. Separable Bell-diagonal states are those with positive partial transpose [2]. Partial transposition changes the sign of c_2, so operators with positive partial transpose occupy the reflection of $\mathcal{T}$ through the plane $c_2 = 0$; the region of separable Bell-diagonal states is the intersection of the two tetrahedra, which is the octahedron $\mathcal{O}$ of Fig. 1 [16].

The entanglement of formation $\mathcal{E}$ [2,17] is a monotonically increasing function of Wootters's concurrence C [17], which for Bell-diagonal states is given by $C = \max(0, 2\lambda_{\max} - 1)$, where $\lambda_{\max} = \max \lambda_{ab}$. The concurrence and the entanglement of formation are convex functions on $\mathcal{T}$. They are zero for the separable states in the octahedron $\mathcal{O}$. In each of the four entangled regions outside $\mathcal{O}$, C and $\mathcal{E}$ are constant on planes parallel to the bounding face of $\mathcal{O}$ and increase as one moves outward through these planes toward the Bell-state vertex.

Quantum discord was introduced by Ollivier and Zurek [7]. We restrict attention to it because of its prominence among measures of nonclassical correlations and because it has been a focus of recent work on decoherence and nonclassical correlations [5,13–15].

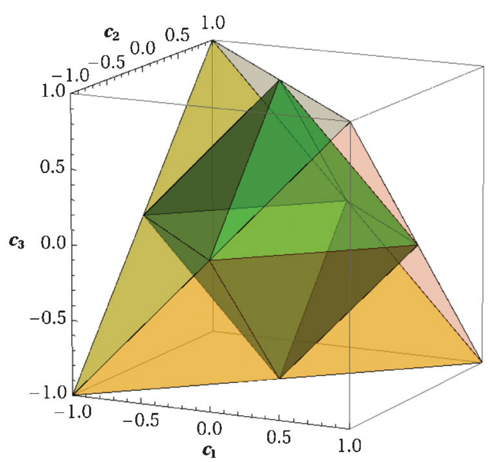

FIG. 1 (color). Geometry of Bell-diagonal states. The tetrahedron $\mathcal{T}$ is the set of valid Bell-diagonal states. The Bell states $|\beta_{ab}\rangle$ sit at the four vertices, the extreme points of $\mathcal{T}$. The green octahedron $\mathcal{O}$, specified by $|c_1| + |c_2| + |c_3| \leq 1$ ($\lambda_{ab} \leq 1/2$), is the set of separable Bell-diagonal states. There are four entangled regions outside $\mathcal{O}$, one for each vertex of $\mathcal{T}$, in each of which the biggest eigenvalue λ_{ab} is the one associated with the Bell state at the vertex. Classical states, i.e., those diagonal in a product basis, lie on the Cartesian axes.

To define quantum discord, one starts with the quantum mutual information, $\mathcal{I} = S(\rho_A) + S(\rho_B) - S(\rho_{AB}) = S(\rho_B) - S(B|A)$, where $S(\rho) = -\mathrm{tr}(\rho \log_2 \rho)$ is the von Neumann entropy of ρ and $S(B|A) = S(\rho_{AB}) - S(\rho_A)$ is a conditional quantum entropy. The quantum mutual information is regarded as quantifying the *total* correlations in the joint state ρ_{AB}.

The quantum mutual information of Bell-diagonal states,

$$\mathcal{I} = 2 - S(\rho_{AB}) = \sum_{a,b} \lambda_{ab} \log_2(4\lambda_{ab}), \quad (3)$$

is a convex function on $\mathcal{T}$. It has smooth level surfaces that bulge outward toward the vertices of $\mathcal{T}$.

The next step is to quantify *purely classical* correlations in terms of information from measurements. One imagines measuring on A a positive-operator-valued measure (POVM) consisting of rank-one POVM elements $E_k = Dq_k|k\rangle\langle k|$ [18], where D is the dimension of A and the q_k make up a normalized probability distribution. The probability to get result k is $p_k = Dq_k\langle k|\rho_A|k\rangle$, and the post-measurement state of B is $\rho_{B|k} = \langle k|\rho_{AB}|k\rangle / \langle k|\rho_A|k\rangle$. Minimizing the average entropy of B, given result k, over measurements on A, yields a classical conditional entropy

$$\tilde{S}(B|A) \equiv \min_{\{E_k\}} \sum_k p_k S(\rho_{B|k}); \quad (4)$$

minimizing chooses the measurement of A that extracts as much information as possible about B. The corresponding mutual-information-like quantity $\mathcal{C} = S(\rho_B) - \tilde{S}(B|A)$ is the measure of classical correlations.

For Bell-diagonal states, we have

$$\mathcal{C} = 1 - H_2\left(\frac{1+c}{2}\right) = \frac{1+c}{2}\log_2(1+c) + \frac{1-c}{2}\log_2(1-c), \quad (5)$$

where $H_2(p) = -p\log_2 p - (1-p)\log_2(1-p)$ is the binary entropy and $c = \max|c_j|$ [19,20]. This $\mathcal{C}$, a convex function on $\mathcal{T}$, is constant on the surfaces of cubes (or the portion of such a cube in $\mathcal{T}$) centered at the origin of Fig. 1—this introduces nonanalyticity—and $\mathcal{C}$ increases monotonically with the size of the cube.

Discord is defined as the difference of $\mathcal{I}$ and $\mathcal{C}$,

$$\mathcal{D} = \mathcal{I} - \mathcal{C} = \tilde{S}(B|A) - S(B|A), \quad (6)$$

thus capturing a notion of nonclassical correlations. Since $\mathcal{C}$ is generally asymmetric between A and B, so also is the discord; this means, in particular, that discord, as defined, vanishes if and only if ρ_{AB} is diagonal in a conditional product basis $|e_j^A\rangle \otimes |f_{jk}^B\rangle$, rather than only in a product basis $|e_j^A\rangle \otimes |f_k^B\rangle$. Bell-diagonal states being symmetric between A and B, however, discord is zero only for classical states, which lie on the Cartesian axes in Fig. 1 [12].

Figure 2 plots level surfaces of discord for Bell-diagonal states. From these plots, it is clear that discord is quite different from entanglement of formation, quantum mutual information, and the measure of classical correlations. Whereas $\mathcal{E}$, $\mathcal{I}$, and $\mathcal{C}$ generally increase outward from the origin, $\mathcal{D}$ increases away from the Cartesian axes, capturing an entropic notion of distance from classical states [9,12]. In particular, as one moves outward along one of the constant-discord tubes of Fig. 2, the classical correlations and the total correlations of the quantum mutual information increase, but their difference, the nonclassical correlations as measured by discord, remains constant. At the vertices of $\mathcal{O}$, $\mathcal{I} = \mathcal{C} = 1$ and $\mathcal{D} = \mathcal{E} = 0$. At the Bell-state vertices of $\mathcal{T}$, $\mathcal{I} = 2$ and $\mathcal{C} = \mathcal{D} = \mathcal{E} = 1$, this being the maximum value of discord for two qubits. In addition, $\mathcal{E}$, $\mathcal{I}$, and $\mathcal{C}$ are all convex, whereas discord is neither concave nor convex, as is evident from the plots in Fig. 2: one can mix two positive-discord states to get a zero-discord classical state, and one can mix two zero-discord classical states on different axes to get a positive-discord state [21].

Mazzola, Piilo, and Maniscalco [15] recently investigated the dynamics of classical and nonclassical correlations, as measured by discord, for two qubits under decoherence processes that preserve Bell-diagonal states. In particular, they considered independent phase-flip channels for the two qubits. The phase flips are implemented mathematically by random applications of σ_z operators to the qubits. This decoherence process leaves c_3 unchanged, but flips the signs of c_1 and c_2 randomly, leading to exponential decay of c_1 and c_2 at the same rate. Mazzola and collaborators found that for the initial conditions they considered, the entanglement of formation decays to zero in a finite time—sudden death of entanglement [4]—but that the discord remains constant for a finite time and then decays, reaching zero at infinite time. This situation is depicted in terms of the surfaces of constant discord in Fig. 3. The decohering-state trajectory is a straight line that runs along a tube of constant discord, until it encounters an intersecting tube, after which the discord decreases to zero when the state becomes fully classical.

This behavior is generic for flip channels and initial conditions on edges of the state tetrahedron. We focus here on the phase-flip channel with initial conditions in the $(+, -, +)$ octant, but analogous considerations apply to the other flip channels (bit and bit phase) and to initial conditions on the other edges of $\mathcal{T}$. Consider then initial conditions anywhere along the edge of $\mathcal{T}$ in this octant: $c_1(0) = 1$ and $0 \leq -c_2(0) = c_3(0) \leq 1$. The trajectory under phase flips is a straight line $c_3 = c_3(0) = -c_2/c_1$. Along this straight line, the eigenvalues λ_{ab} factor into products of probabilities, $(1 \pm c_1)/2$ and $(1 \pm c_3)/2$, thus making $S(\rho_{AB})$ the entropy of two independent binary random variables with these probabilities. This yields a quantum mutual information $\mathcal{I} = 2 - H_2[(1 + c_3)/2] -$

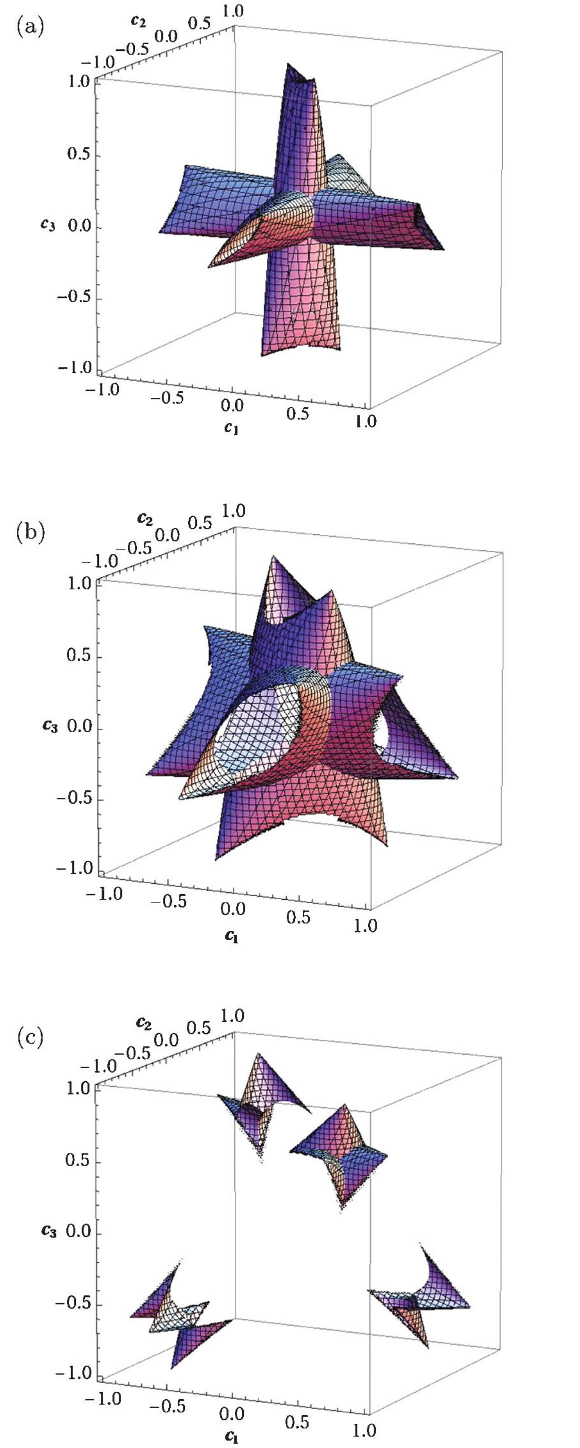

FIG. 2 (color). Surfaces of constant discord, (a) $\mathcal{D} = 0.03$, (b) $\mathcal{D} = 0.15$, (c) $\mathcal{D} = 0.35$. The level surfaces consist of three intersecting "tubes" running along the three Cartesian axes. The tubes are cut off by the state tetrahedron $\mathcal{T}$ at their ends, and they are squeezed and twisted so that at their ends they align with an edge of $\mathcal{T}$. As discord decreases, the tubes collapse to the Cartesian axes [12]. As discord increases, the tube structure is obscured, as in (c): the main body of each tube is cut off by $\mathcal{T}$; all that remain are the tips, which reach out toward the Bell-state vertices.

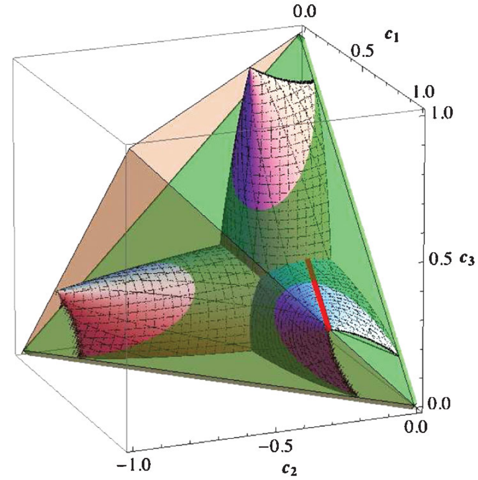

FIG. 3 (color). Trajectory (red) of a Bell-diagonal state under random phase flips of the two qubits; initial conditions are $c_1(0) = 1$, $-c_2(0) = c_3(0) = 0.3$. The trajectory is the straight line $c_3 = c_3(0) = 0.3 = -c_2/c_1$. For clarity, only the $(+, -, +)$ octant is shown. A constant-discord surface is plotted for the discord value of the initial state. Faces of the yellow state tetrahedron $\mathcal{T}$ and the green separable octahedron $\mathcal{O}$ are also shown. The straight line trajectory proceeds along a tube of constant discord till it encounters the vertical tube at $c_1 = 0.3$, after which discord decreases monotonically to zero when the trajectory reaches the c_3 axis. Entanglement of formation decreases monotonically to zero when the trajectory enters $\mathcal{O}$ at $c_1 = 0.7/1.3 = 0.54$.

$H_2[(1 + c_1)/2]$. Furthermore, along the trajectory $c = \max(c_1, c_3)$. The result is that the trajectory initially runs along a tube of constant discord

$$\mathcal{D} = 1 - H_2\left(\frac{1 + c_3}{2}\right), \qquad (7)$$

for $c_1 \geq c_3$. When $c_1 = c_3$, the trajectory encounters another tube, after which, for $c_1 \leq c_3$, the discord decreases monotonically as $\mathcal{D} = 1 - H_2[(1 + c_1)/2]$ as c_1 decreases. Meanwhile, the entanglement of formation decreases monotonically from its initial value to a sudden death at $c_1 = (1 - c_3)/(1 + c_3)$.

The situation investigated in [15] is surely interesting: under decoherence, nonclassical correlations remain constant for a finite time interval. This situation is, however, a special one, as can be seen from the surfaces of constant discord; the trajectories considered here are the only straight lines in parameter space that stay on a surface of constant discord. Indeed, the pictorial approach can provide a complete understanding of how entanglement and nonclassicality change under decoherence within the set of Bell-diagonal states.

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*mlang@unm.edu

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[21] This argument and its conclusion are not special to Bell-diagonal states: mixing two discordant states can lead to a state that is diagonal in a product basis, and mixing two states that are diagonal in incompatible product bases generally leads to a discordant state.